

PAIR FORMATION IN A t -J MODEL

COURSE PH-614

M.Sc. Project Report II

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CERTIFICATE

It is certified that the work contained in the project titled **Pair Formation in a t-J Model** has been carried out by Ayan Khan, under my supervision.

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Contents

1	INTRODUCTION:	2
2	MANY PARTICLE SYSTEM:	3
2.1	Second Quantization:	3
2.2	Theoretical Models in Many Particle Systems:	5
2.2.1	Tight Binding Model:	5
2.2.2	Heisenberg Model:	5
2.2.3	Hubbard Model:	5
2.2.4	t-J-U Model	6
2.3	Construction of Equation of Motion (EOM) for Two Particle System:	7
3	CALCULATIONS:	8
3.1	One Dimensional Chains:	8
3.2	Two Dimensional Square Lattice:	11
3.3	Two Leg Ladder:	15
3.4	Three Dimensional Cubic Lattice:	17
4	RESULTS AND DISCUSSION:	21
5	CONCLUSION AND FUTURE PROSPECTS:	23

ABSTRACT

We have investigated the formation of bound state of two electrons in different kind of lattices using a t-J-U model. In the model hopping parameter t tries to delocalize the electrons where as pairing of electrons comes via Heisenberg exchange integral J and hence it becomes necessary to calculate the threshold value of J , viz. J_c , for which formation of bound states between two electron system is possible. The analysis is repeated for one dimensional chains, two dimensional square lattices, two leg ladders and three dimensional simple cubic lattices. Further we calculated the bound state energies for $J > J_c$. Also we have tried to shed some light to the symmetry operation of the lattices to understand the characteristic of two electron pairing.

1 INTRODUCTION:

The discovery of superconductivity in 1911 by Kammerlingh Onnes had given a new dimension in Condensed Matter Physics research. From the very beginning the scientific and commercial potential of superconductors had been well understood by the community. So as the days progressed different exciting features of superconductivity started to come to light and in 1987 with the discovery of high temperature superconductors the field of interest is further broadened.

Normal superconductors, which are usually good metals, are quite well understood by BCS theory where electron electron interaction is mainly controlled by phonons. But in high temperature superconductors the interaction picture among the electrons are still not clear.

Here our motivation is to study strongly correlated systems because it is well agreed that the origin of high temperature superconductivity is purely from electronic interaction, as for example here we are interested to study two dimensional square lattice which is analogous to the CuO_2 planes in a high temperature superconductor.

There are several models to study many particle systems and we are here using t-J model for studying electron pairing in metals with t denoting kinetic energy and J denoting Heisenberg exchange integral. We are starting with the assumption that the parent compounds are quite well represented by the antiferromagnetic Heisenberg model with localized electrons of spin 1/2 occupying a lattice point and coupled by an exchange integral J. Doping is assumed to remove electrons thereby producing "holes" which are mobile because neighboring electrons can hop to the hole site with amplitude t. It has been shown earlier that [1] for the t-J model, dilute holes in an antiferromagnet are unstable against phase separation into a hole rich and a no hole phase. It can be argued that there exists a critical value of J_c , such that when spin exchange integral J exceeds J_c , the hole rich phase has no electrons and for J slightly less than J_c the hole rich phase is a low density superfluid of electron pairs.

Here we are investigating the critical value of J for which pairing of electron is possible in different kind of lattices. On the due course in the earlier semester we had concentrated on one dimensional chains. One dimensional analysis always carries a significant importance for its relative simplicity, also if one dimensional lattice features are well understood then it becomes relatively easy to understand the higher dimensional lattices. Then we had taken one step ahead to two dimensional square lattice. As we have stated the features of the two dimensional lattice has become very important after the discovery of high temperature superconductors in ceramic materials. The structural feature of ceramic materials is CuO_2 plane which are the main source for high temperature superconductivity. So it is important to understand the electron correlation in two dimensional lattices. Further we had extended our study on two leg ladder lattice. Since for the one-dimensional chain system quite a few things are known exactly. One approach to tackle the superconducting cuprates is to investigate the quasi one-dimensional lattices known as 'spin ladder' structures, which are strips of square lattice with a finite width and infinite length. An example of spin ladder lattice system is $Sr_{n-1}Cu_{n+1}O_{2n}$. For these above mentioned lattices we had verified

the critical value of J in square lattice which is $2t$ [2]. Also we had investigated the critical value for one dimensional chain like lattice and two leg ladder where again we land up with the same result as $J = 2t$.

In this semester we were curious to look at the critical value of J in a simple cubic lattice. To understand the electronic interaction of the heavy-fermionic superconductors such as $CeCu_2Si_2$, one needs to deal with different three dimensional crystal structures. So it is a natural to look at a three dimensional structure and try to find out the critical value of J for which pair formation among two electrons is possible. So we calculated J_c for a simple cubic lattice and this constitutes a new and central result in this project work.

2 MANY PARTICLE SYSTEM:

2.1 Second Quantization:

To understand the many body theory in condensed matter physics the essential technique is the method of second quantization. Soon after the foundation of quantum theory, the formalism of creation and annihilation operator (second quantization) was introduced. The physics of creation and annihilation operators can be explained in a better way from relativistic quantum field theory. So second quantization is nothing but a alternative formulation of quantum mechanics. the creation and annihilation operators are nothing but a tool that permits different process such as creation and annihilation of operators. Such process can not be discussed in the framework of Schrödinger equation[3].

We know that quantum mechanical wave function which represents a collection of electrons is antisymmetric with respect to the operation which exchanges the space and spin coordinates of any two electrons. Thus, if $\psi(1, 2, 3, \dots, N)$ is an N electron wave function, and if P_{ij} is the operator which exchanges the coordinates if electron i and electron j , then $P_{ij}\Psi = -\Psi$

J. C. Slater has introduced a method to represent such many electron wave functions. We need to begin with an orthonormal set of one-electron functions: ϕ_1, ϕ_2, \dots , where $\int d\tau_1 \phi_i^*(1)\phi_j(1) = \delta_{ij}$ [3], where

$$\Delta = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(r_1) & \dots & \dots & \phi_1(r_N) \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \phi_N(r_1) & \dots & \dots & \phi_N(r_N) \end{vmatrix} \equiv |\phi_1\phi_2\phi_3\dots|$$

Such a function is called "Slater determinant." Since interchange of any two columns of a determinant changes its sign, Δ is antisymmetric with respect to the exchange operator P_{ij} .

We can also represent antisymmetric many electron wave function in a different manner. Let us now define a set of electron creation operators, $b_1^\dagger, b_2^\dagger, \dots$, corresponding to the one electron spin orbitals, ϕ_1, ϕ_2, \dots . When the creation operator b_j^\dagger acts on

an N-electron state, it produces an (N+1) electron state by creating an electron in the spin-orbital ϕ_j . We used to denote no electron state or "vacuum state" as $|0\rangle$. Similarly we define annihilation operator as b_j .

The commutation relations of the operators as follows:

$$\begin{aligned} b_j|0\rangle &= 0, \quad \langle 0|b_j^\dagger = 0 \\ |b_j|N\rangle &= |N-1\rangle, \quad b_j^\dagger|N\rangle = 0 \\ b_i^\dagger b_j + b_j b_i^\dagger &= \delta_{ij} \\ b_i^\dagger b_j^\dagger + b_j^\dagger b_i^\dagger &= 0 \\ b_i b_j + b_j b_i &= 0 \end{aligned}$$

Now we can also represent Slater determinant with creation and annihilation

$$\begin{aligned} \text{operators, } \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) \\ \phi_2(r_1) & \phi_2(r_2) \end{vmatrix} &\equiv |\phi_1\phi_2\rangle = b_i^\dagger b_j^\dagger |0\rangle \\ \text{Also } b_i^\dagger b_j^\dagger |0\rangle &= -b_j^\dagger b_i^\dagger |0\rangle \end{aligned}$$

Now we can write kinetic energy operator as

$$\hat{T} = \sum_{i,j} \langle i|T|j\rangle b_i^\dagger b_j$$

Similarly, the potential energy operator can be written as,

$$\hat{V} = \frac{1}{2} \sum_{i,j,k,l} \langle ij|V(\mathbf{r}_1, \mathbf{r}_2)|kl\rangle b_i^\dagger b_j^\dagger b_l b_k$$

Now if we define field operator as

$$\begin{aligned} \Psi(\mathbf{r}) &= \sum_i b_{n_i} \phi_{n_i}(\mathbf{r}) \\ \Psi^\dagger(\mathbf{r}) &= \sum_i b_{n_i}^* \phi_{n_i}^\dagger(\mathbf{r}) \end{aligned}$$

then

$$\begin{aligned} \langle i|\hat{T}|j\rangle &= \int d^3r \phi_{n_i}^\dagger(r) T(r) \phi_{n_j}(r) \\ \langle ij|\hat{V}|kl\rangle &= \int \int d^3r_1 d^3r_2 \phi_{n_i}^\dagger(r_1) \phi_{n_j}^\dagger(r_2) V|r_1 - r_2| \phi_{n_k}(r_1) \phi_{n_l}(r_2) \end{aligned}$$

If we consider Bloch wave function i.e $\phi(\mathbf{r}) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} u_{kn}(\mathbf{r})$, where $u_{kn}(\mathbf{r})$ signifies particle is in periodic potential the Hamiltonian will be,

$$\hat{H} = \sum_{k,\sigma} \epsilon_k b_{k\sigma}^\dagger b_{k\sigma} + \frac{1}{2} \sum_{q,\sigma,\sigma'} V_q b_{k-q,\sigma}^\dagger b_{k'+q,\sigma} b_{k'\sigma'} b_{k\sigma}$$

this is second quantized Hamiltonian in many electron system.

As for example if we consider $\epsilon_k = -t \sum_\sigma e^{i\mathbf{k}\cdot\delta}$, where t is hopping strength and δ is nearest neighbour where a electron can hop. If our system is a two dimensional square

lattice with lattice parameter \mathbf{a} then, $\delta = \pm\hat{x}a, \pm\hat{y}a$,
 So our energy dispersion relation will be then

$$\epsilon_k = -t(e^{\pm ikx} + e^{\pmiky}) = -2t(\cos k_x + \cos k_y)$$

2.2 Theoretical Models in Many Particle Systems:

2.2.1 Tight Binding Model:

In tight binding model the Hamiltonian describes the kinetic energy (hopping) of electrons for nearest neighbour pairs.

$$\widehat{H} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma})$$

In this approximation we consider the wave function of the electrons are sharply localized neglecting any overlap between them and they are confined in the lattice sites by an infinite potential barrier[4]. From here on we like to fix the notation of creation and annihilation operator as c_i, c_j^\dagger respectively.

2.2.2 Heisenberg Model:

The simplest model in quantum many body theory is isotropic spin half Heisenberg chain. The Heisenberg Hamiltonian is given by:

$$\widehat{H} = J \sum_{\langle i,j \rangle} (\mathbf{S}_i \mathbf{S}_j - \frac{1}{4})$$

where \mathbf{S}_j is a local spin variable at j^{th} state. For antiferromagnets $J > 0$. The sum is over the distinct nearest neighbours. For spin 1/2 particle the spins are represented by Pauli's spin matrices.

2.2.3 Hubbard Model:

The Hubbard model describes the strongly correlated electron systems. The model in more than one dimension has not been solved. In describing the CuO_2 planes in high temperature superconductivity Hubbard model is a good starting point[5]. The basic ingredients of Hubbard model are:

- The kinetic energy (electron hopping) delocalizes the electron in Bloch state, leading to metallic behavior.[6]
- The electron electron interaction (approximated by onsite Coulomb interaction) wants to localize the electron on to sites.[6]

The Hubbard model contains only one orbital per site and is defined as (considering nearest and next nearest neighbour interactions)[5]:

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) - t' \sum_{\langle i,i' \rangle, \sigma} (c_{i\sigma}^\dagger c_{i'\sigma} + c_{i'\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

If we only take into account the nearest neighbour interaction it reduces to:

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

where $c_{i\sigma}^\dagger$ are creation operators and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ are occupation number operator. By means of on site Coulomb U the singlet band of the Hubbard model is split into a lower (LHB) and an upper Hubbard band (UHB). But the validity of the three band model to the single band model is still controversial [5]. It has been questioned whether the strong coupling version of the Hamiltonian, i.e the t-J model, is appropriate to describe correctly the low energy physics of the original three band model. In the large U limit and at half filling (one electron per site) the Hubbard ladder is equivalent to the spin 1/2 Heisenberg ladder [7].

$$\widehat{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

When the Hubbard ladder is doped with holes away from half filling, its strong coupling description is modified from the Heisenberg model to the t-J model with the constrain of no doubly occupied sites[7].

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j)$$

2.2.4 t-J-U Model

The most important local interactions in a doped antiferromagnet are well represented by the large U Hubbard model, the t-J model, and their various relatives. To be concrete we will focus on the t-J-U model. The t-J-U Hamiltonian is written as:

$$\widehat{H} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

It is a close variant of the familiar t-J model where the sites of the lattice is strictly prohibited against double occupancy, i.e the doubly occupied sites are projected out. The "no double occupancy" restriction is suitably achieved by using "constrained" fermionic operators. The same physics can be achieved by using a t-J-U model given by the limit $U \rightarrow \infty$ we go back to simple t-J model. The exchange integral J arises through virtual processes where in the intermediate state has a doubly occupied site, producing an antiferromagnetic coupling. Dopping is assumed to remove electrons thereby producing a "hole" or missing spin which is mobile because neighbouring electrons can hop into its place with amplitude t . So among the other models to study the correlation effects in the high temperature superconductors this model is simplest one and gives a exact critical value of $J(J_c)$ such that $J \geq J_c$ two electrons can form a two particle bound state.

2.3 Construction of Equation of Motion (EOM) for Two Particle System:

The system consisting of two electrons the wave function can be written as

$$|\Psi\rangle = \sum_{i_1, i_2} \Phi(i_1, i_2) c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle \quad (1)$$

and the model Hamiltonian is

$$\hat{H} = -t \sum_{\langle i, j \rangle} \sum_{\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + J \sum_{\langle i, j \rangle} (S_i \cdot S_j - \frac{n_i \cdot n_j}{4}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (2)$$

where $|0\rangle$ denotes the vacuum state. For a two body problem the ground state is a singlet i.e $\Phi(i_1, i_2) = \Phi(i_2, i_1)$ and we know that $H|\Psi\rangle = E|\Psi\rangle$ so the equation of motion can be written as

$$[-t \sum_{\langle i, j \rangle} \sum_{\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + J \sum_{\langle i, j \rangle} (S_i \cdot S_j - \frac{n_i \cdot n_j}{4}) + U \sum_i n_{i\uparrow} n_{i\downarrow}] \sum_{i_1, i_2} \Phi(i_1, i_2) c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle = E \sum_{i_1, i_2} \Phi(i_1, i_2) c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle \quad (3)$$

$$\begin{aligned} \hat{t}|\Psi\rangle &= -t \sum_{\langle i, j \rangle} \sum_{\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \sum_{i_1, i_2} \Phi(i_1, i_2) c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle \\ &= -t \sum_{\langle i, j \rangle} \sum_{i_1, i_2} \Phi(i_1, i_2) (c_{i_1\uparrow}^\dagger c_{j\uparrow} c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle + c_{j\uparrow}^\dagger c_{i_1\uparrow} c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle + c_{i_1\downarrow}^\dagger c_{j\downarrow} c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle + c_{j\downarrow}^\dagger c_{i_1\downarrow} c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle) \\ &= \sum_j \Phi(j, i_2) c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle + 0 - \sum_j \Phi(i_1, j) c_{i_1\downarrow}^\dagger c_{i_2\uparrow}^\dagger |0\rangle + 0 \\ \hat{t}|\Psi\rangle &= -t [\sum_j \Phi(j, i_2) c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle - \Phi(i_1, j) c_{i_1\downarrow}^\dagger c_{i_2\uparrow}^\dagger |0\rangle] \end{aligned} \quad (4)$$

$$\begin{aligned} \hat{U}|\Psi\rangle &= U \sum_{\langle i, j \rangle} \sum_{i_1, i_2} \Phi(i_1, i_2) c_{i_1\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i_2\downarrow}^\dagger c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle \\ &= U \sum_{i_1, i_2} \Phi(i_1, i_2) \delta_{i_1 i_2} c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle \end{aligned} \quad (5)$$

$$\begin{aligned} \hat{J}|\Psi\rangle &= J \sum_{\langle i, j \rangle} \sum_{i_1, i_2} \Phi(i_1, i_2) (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i \cdot n_j}{4}) c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle \\ &= J \sum_{i_1, i_2} \Phi(i_1, i_2) c_{i_1\uparrow}^\dagger c_{i_2\downarrow}^\dagger |0\rangle \end{aligned} \quad (6)$$

$$E\Phi(i_1, i_2) = \sum_j [t_{i_1 j} \Phi(j, i_2) + t_{i_2 j} \Phi(i_1, j)] + [U \delta_{i_1, i_2} - J_{i_1, i_2}] \Phi(i_1, i_2) \quad (7)$$

Fourier transform of the equation yields

$$E\Phi(\mathbf{k}_1, \mathbf{k}_2) = [t(\mathbf{k}_1) + t(\mathbf{k}_2)] \Phi(\mathbf{k}_1, \mathbf{k}_2) + \frac{U}{N} \sum_{\mathbf{k}} \Phi(\mathbf{k}_1 + \mathbf{k}, \mathbf{k}_2 - \mathbf{k}) - \frac{1}{N} \sum_{\mathbf{k}} J(\mathbf{k}) \Phi(\mathbf{k}_1 - \mathbf{k}, \mathbf{k}_2 + \mathbf{k}) \quad (8)$$

where,

$$\begin{aligned}\Phi(\mathbf{k}_1, \mathbf{k}_2) &= \frac{1}{N} \sum_{i_1, i_2} \Phi(i_1, i_2) e^{-i\mathbf{k}_1 \cdot \mathbf{r}_{i_1} - i\mathbf{k}_2 \cdot \mathbf{r}_{i_2}} \\ t(\mathbf{k}) &= \frac{1}{N} \sum_{i,j} t_{ij} e^{-\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} = -2t(\cos k_x + \cos k_y) \\ J(\mathbf{k}) &= 2J(\cos k_x + \cos k_y)\end{aligned}$$

taking the lattice constant 1. Since the system is translationally invariant, the total momentum can be used to specify its eigenstates. let us define $\mathbf{Q} = \mathbf{k}_1 + \mathbf{k}_2$, $\mathbf{q} = \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$, and $\Phi(\mathbf{k}_1, \mathbf{k}_2) = \Phi_Q(\mathbf{q})$ then we obtain

$$\Phi_Q(\mathbf{q}) = \frac{\frac{U}{N} \sum_k \Phi_Q(\mathbf{k}) - \frac{1}{N} \sum_k J(\mathbf{q} - \mathbf{k}) \Phi_Q(\mathbf{k})}{E - t(\frac{\mathbf{Q}}{2} + \mathbf{q}) - t(\frac{\mathbf{Q}}{2} - \mathbf{q})} \quad (9)$$

This is the starting point of our analysis.

3 CALCULATIONS:

3.1 One Dimensional Chains:

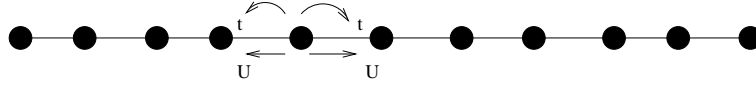


Fig 1

For singlet pairing we can take $Q=0$ so from eq. (9) can be decoupled so that we can write,

$$C_0 = UC_0 I_0 - 2JI_x C_x \quad (10)$$

$$C_x = UC_0 I_x - 2JI_{xx} C_x \quad (11)$$

where

$$\begin{aligned}C_0 &= \frac{1}{N} \sum_{\mathbf{q}} \Phi_0(\mathbf{q}) \\ C_x &= \frac{1}{N} \sum_k \cos k_x \Phi_0(\mathbf{k}) \\ I_0 &= \frac{1}{N} \sum_q \frac{1}{E + 4t \cos q_x} \\ I_x &= \frac{1}{N} \sum_q \frac{\cos q_x}{E + 4t \cos q_x}\end{aligned}$$

$$I_{xx} = \frac{1}{N} \sum_q \frac{\cos^2 q_x}{E + 4t \cos q_x}$$

eq. (11) and (12) can be written in matrix form as follows:

$$\begin{pmatrix} UI_0 - 1 & -2JI_x \\ UI_x & -2JI_{xx} - 1 \end{pmatrix} \begin{pmatrix} C_0 \\ C_x \end{pmatrix} = 0 \quad (12)$$

In eq. (12) unique solution of C_0 and C_x will exist if and only if the determinant of the coefficient is zero.

$$\begin{vmatrix} UI_0 - 1 & -2JI_x \\ UI_x & -2JI_{xx} - 1 \end{vmatrix} = 0 \quad (13)$$

Now solving eq. (13) for J

$$-2J = \frac{1 - UI_0}{I_x^2 U + I_{xx}(1 - UI_0)} \quad (14)$$

Using the lattice symmetry we can write

$$\begin{aligned} I_0 &= -\frac{1}{4} \frac{1}{\sqrt{\alpha^2 - 1}} \\ I_x &= \frac{1}{4} \frac{\alpha + \sqrt{\alpha^2 - 1}}{\sqrt{\alpha^2 - 1}} \\ I_{xx} &= -\frac{1}{4} \frac{\alpha(\alpha + \sqrt{\alpha^2 - 1})}{\sqrt{\alpha^2 - 1}} \end{aligned}$$

eq. (15), (16), (17) can be written in a more simple form as

$$I_x = \frac{1}{4t} - \frac{E}{4t} I_0 \quad (15)$$

$$I_{xx} = -\frac{E}{4t} I_x \quad (16)$$

substituting these values with the limit as $I_0 \rightarrow \infty$ and $U \rightarrow \infty$ in eq. (14) we get $\mathbf{J_c = 2t}$

Bound state energy of electron in one dimension

If we think in terms of the energy band in one dimension it is $8t$ for our system, so the bound state energy E of the two particle system can be obtained via equation (14), (15), (16) is we can write

$$\frac{8t}{J} = \frac{1}{tI_0} - \frac{E}{t} \quad (17)$$

Taking $t = 1$ we can write the energy equation as

$$E = \frac{1}{I_0} - \frac{8t^2}{J} \quad (18)$$

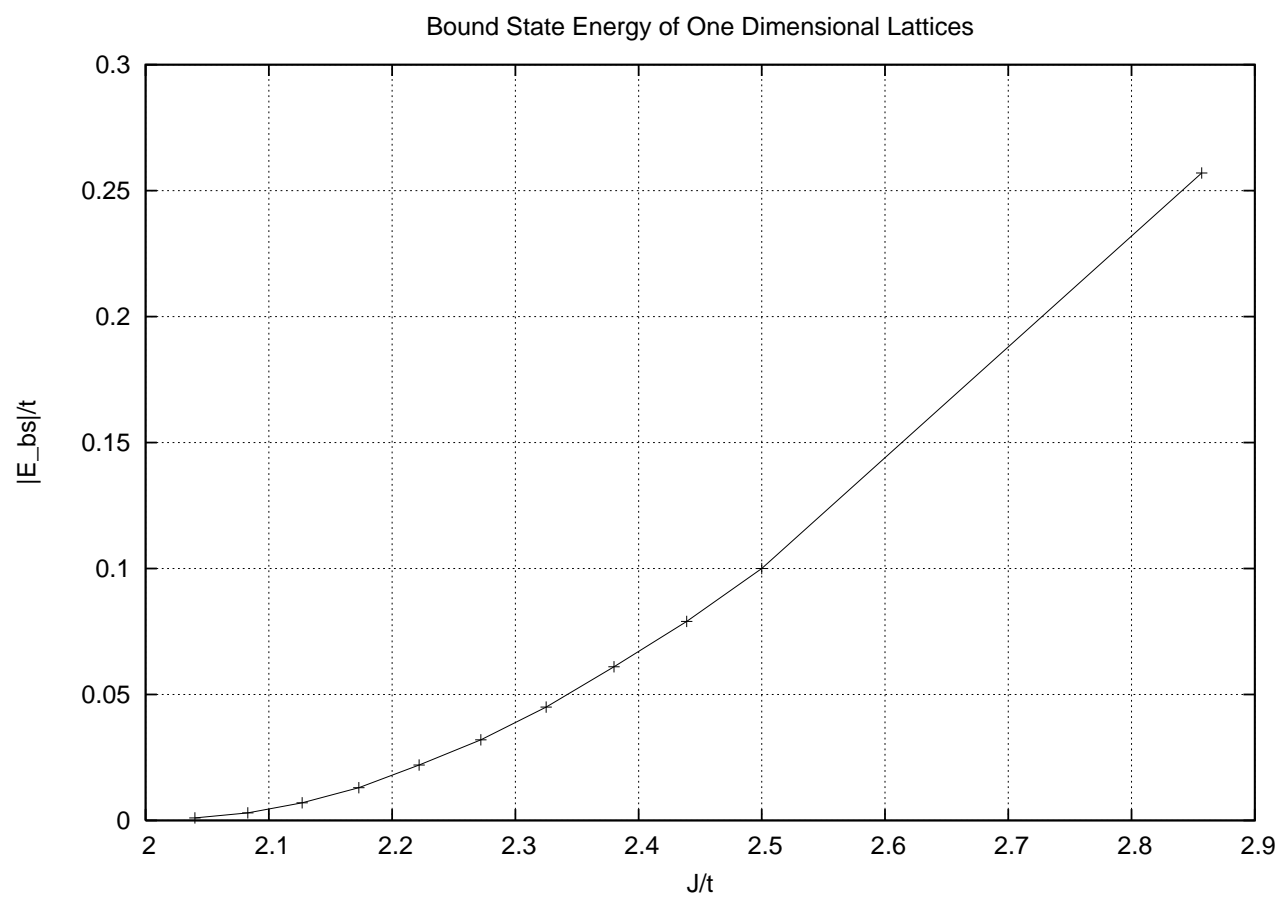


Fig 2

3.2 Two Dimensional Square Lattice:

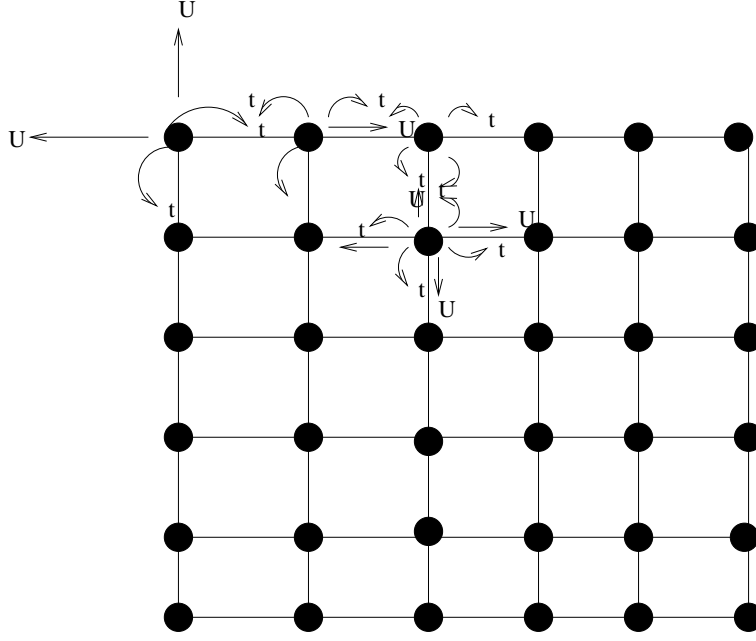


Fig 3

In a similar fashion as we have done in the previous section we can write the following equations:

$$C_0 = UI_0C_0 - 2JI_xC_x - 2JI_yC_y \quad (19)$$

$$C_x = UC_0I_x - 2JC_xI_{xx} - 2JC_yI_{xy} \quad (20)$$

$$C_y = UC_0I_y - 2JC_xI_{xy} - 2JC_yI_{yy} \quad (21)$$

where

$$C_0 = \frac{1}{N} \sum_{\mathbf{q}} \Phi_0(\mathbf{q})$$

$$C_x = \frac{1}{N} \sum_k \cos k_x \Phi_0(\mathbf{k})$$

$$C_y = \frac{1}{N} \sum_k \cos k_y \Phi_0(\mathbf{k})$$

$$I_0 = \frac{1}{N} \sum_q \frac{1}{E + 4t(\cos q_x + \cos q_y)}$$

$$I_x = \frac{1}{N} \sum_q \frac{\cos q_x}{E + 4t(\cos q_x + \cos q_y)}$$

$$\begin{aligned}
I_{xx} &= \frac{1}{N} \sum_q \frac{\cos^2 q_x}{E + 4t \cos q_x} \\
I_y &= \frac{1}{N} \sum_q \frac{\cos q_y}{E + 4t(\cos q_x + \cos q_y)} \\
I_{xy} &= \frac{1}{N} \sum_q \frac{\cos q_x \cos q_y}{E + 4t(\cos q_x + \cos q_y)} \\
I_{yy} &= \frac{1}{N} \sum_q \frac{\cos^2 q_y}{E + 4t(\cos q_x + \cos q_y)}
\end{aligned}$$

eq. (20),(21),(22) can be written in a matrix form as follows:

$$\begin{pmatrix} UI_0 - 1 & -2JI_x & -2JI_y \\ UI_x & -2JI_{xx} - 1 & -2JI_{xy} \\ UI_y & -2JI_{xy} & -2JI_{yy} - 1 \end{pmatrix} \begin{pmatrix} C_0 \\ C_x \\ C_y \end{pmatrix} = 0 \quad (22)$$

In eq. (23) unique solution of C_0 , C_x and C_y will exit if and only if the determinant of the coefficient matrix is zero.

$$\begin{vmatrix} UI_0 - 1 & -2JI_x & -2JI_y \\ UI_x & -2JI_{xx} - 1 & -2JI_{xy} \\ UI_y & -2JI_{xy} & -2JI_{yy} - 1 \end{vmatrix} = 0 \quad (23)$$

For an isotropic square lattice symmetry permits us to write $I_y = I_x$, $I_{yy} = I_{xx}$ and $C_y = C_x$ hence eq. (23) becomes

$$\begin{pmatrix} UI_0 - 1 & -2JI_x & -2JI_x \\ UI_x & -2JI_{xx} - 1 & -2JI_{xy} \\ UI_y & -2JI_{xy} & -2JI_{xx} - 1 \end{pmatrix} \begin{pmatrix} C_0 \\ C_x \\ C_x \end{pmatrix} = 0 \quad (24)$$

and our modified determinant will be,

$$\begin{vmatrix} UI_0 - 1 & -2JI_x & -2JI_x \\ UI_x & -2JI_{xx} - 1 & -2JI_{xy} \\ UI_x & -2JI_{xy} & -2JI_{xx} - 1 \end{vmatrix} = 0 \quad (25)$$

Now our motivation is to take $U \rightarrow \infty$ limit to project out the possibility of double occupancy. The value of I_0, I_x, I_{xx}, I_{xy} after integration are as follows:

$$I_0 = \frac{1}{2} \frac{K(\frac{-2}{\alpha})}{\pi \alpha} \quad (26)$$

$$I_x = \frac{1}{2} \frac{(1 - \alpha)K(\frac{-2}{\alpha})}{\pi \alpha} - \frac{1}{2} \frac{(\alpha - 2)\Pi(\frac{2}{\alpha}, \frac{-2}{\alpha})}{\pi} \quad (27)$$

$$I_{xx} = \frac{1}{4} \frac{(\alpha^2 - 2\alpha + 2)K(\frac{-2}{\alpha})}{\pi \alpha} - \frac{1}{2} \frac{(\alpha - 2)\Pi(\frac{2}{\alpha}, \frac{-2}{\alpha})}{\pi} + \frac{1}{4} \frac{\alpha E(-\frac{2}{\alpha})}{\pi} \quad (28)$$

$$I_{xy} = -\frac{1}{2} \frac{(1-\alpha)K(\frac{-2}{\alpha})}{\pi} - \frac{1}{2} \frac{(\frac{1}{2}\alpha - \alpha + 1)K(-\frac{2}{\alpha})}{\pi\alpha} - \frac{1}{4} \frac{\alpha E(-\frac{2}{\alpha})}{\pi} \quad (29)$$

These expression can be written in a simple form as:

$$I_{xx} + I_{xy} = -\frac{E}{4t} I_x \quad (30)$$

$$I_x = \frac{1}{8t} - \frac{E}{8t} I_0 \quad (31)$$

$$I_0 = \frac{1}{E} \frac{2}{\pi} K\left(\frac{8t}{E}\right) \quad (32)$$

So the lattice integrals are turned out in terms of complete elliptic integral of first kind ($K(k)$), second kind ($E(k)$), third kind ($\Pi(\nu, k)$) respectively. $\Pi(\nu, k)$ can be evaluated through $K(k)$, $E(k)$, $F(q, \phi)$, $E(q, \phi)$, where $F(q, \phi)$ and $E(q, \phi)$ are the incomplete Elliptic integrals of first and second kind respectively[8]. The nature of $K(k)$ and $E(k)$ is shown as follows:

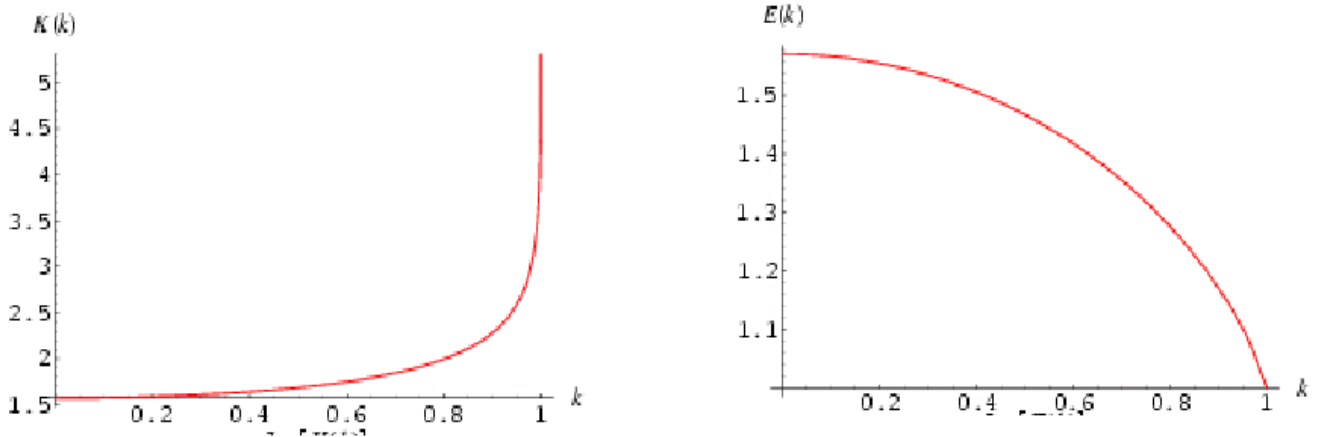


Fig 4

So from the physical nature of the elliptic integral of the first kind we can conclude that it is of logarithmic diverging nature so to tackle this problem let us consider $\alpha = -2 - \delta$ and expand the elliptic integrals w.r.t δ then take $\delta \rightarrow 0$ limit. Since the determinant is zero thus the coefficient of the diverging $\ln \delta$ term should be equal to zero.

$$\text{So } -\frac{1}{32} \frac{J^2}{\pi} + 18 \frac{1}{\pi} - \frac{1}{4} \frac{J}{\pi^2} + \frac{1}{8} \frac{J^2}{\pi^2} = 0$$

The solution of the quadratic equation for $\mathbf{J} = 2t$ and $\mathbf{7.32t}$.

Bound state energy of electron in two dimension

From eq. (24) we can write

$$-2J = \frac{1 - UI_0}{2UI_x^2 + (I_{xx} + I_{xy})(1 - UI_0)} \quad (33)$$

From eq. (31), (32), (33), and (34) the bound state energy E of the two electron system can be obtained via

$$\frac{16t}{J} = \frac{\pi}{2} \frac{\frac{E}{t}}{K(\frac{8t}{E})} - \frac{E}{t} \quad (34)$$

Taking $t = 1$ we rewrite the equation as:

$$E = \frac{16}{J(\frac{2}{\pi} \frac{1}{K(\alpha)} - 1)} \quad (35)$$

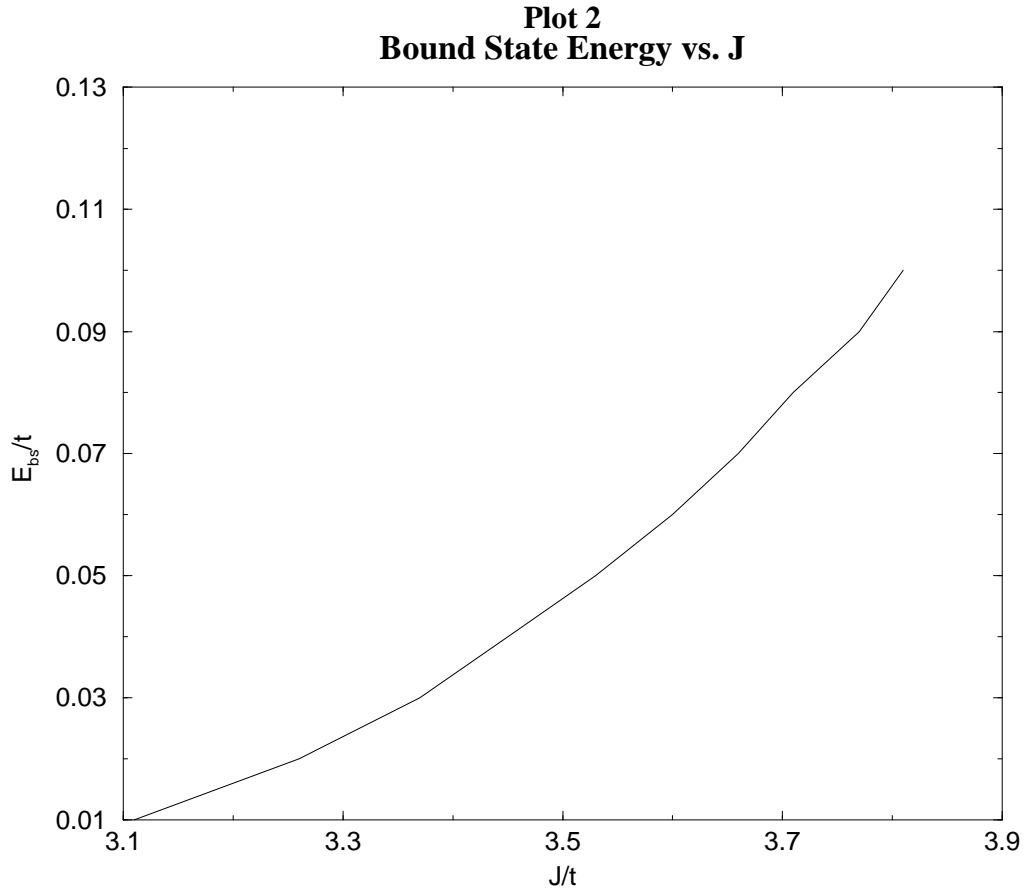


Fig 5

3.3 Two Leg Ladder:

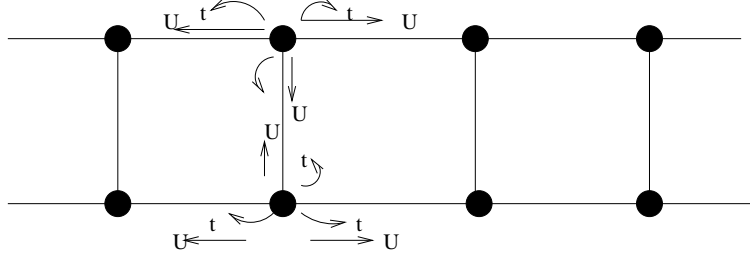


Fig 6

So a ladder like lattice involves a one dimensional wave vector integral (*viz* over q_x) rather than two dimensional integral (over q_x and q_y). More precisely the lattice integrals appearing in the calculation of bound states are expressed as,

$$\sum_q = \frac{1}{2} \sum_{q_y=0,2\pi} \frac{1}{2\pi} \int_{-\pi}^{\pi} dq_x$$

The various lattice integrals are as follows:

$$I_0 = \frac{1}{4} \int_{-\pi}^{\pi} \frac{dx}{\alpha + 1 + \cos q_x} + \frac{1}{4} \int_{-\pi}^{\pi} \frac{dx}{\alpha - 1 + \cos q_x} \quad (36)$$

$$I_x = \frac{1}{4} \int_{-\pi}^{\pi} \frac{\cos q_x dx}{\alpha + 1 + \cos q_x} + \frac{1}{4} \int_{-\pi}^{\pi} \frac{\cos q_x dx}{\alpha - 1 + \cos q_x} \quad (37)$$

$$I_{xx} = \frac{1}{4} \int_{-\pi}^{\pi} \frac{\cos^2 q_x dx}{\alpha + 1 + \cos q_x} + \frac{1}{4} \int_{-\pi}^{\pi} \frac{\cos^2 q_x dx}{\alpha - 1 + \cos q_x} \quad (38)$$

where $\alpha = \frac{E}{4t}$

from eq. (13) with $t = 1$ and $U \rightarrow \infty$ we can write,

$$\begin{vmatrix} I_0 & -2JI_x \\ I_x & -2JI_{xx} - 1 \end{vmatrix} = 0 \quad (39)$$

expanding the determinant we obtain

$$2JI_x^2 - 2JI_0I_{xx} - I_0 = 0 \quad (40)$$

We have substituted the integral values in eq. (42) and also α is replaced by $-\delta - 2$. Then expanding the entire equation w.r.t δ we got a term of $\frac{1}{\sqrt{\delta}}$. This term will diverge as soon as we will take the limit as $\delta \rightarrow 0$. So collecting the coefficients of this term and equating them to zero the critical value of J is obtained which is $2t$.

Bound state energy of Two leg ladder

Directly from the integrals one can find out the bound state energy for pairing of electrons with proper substitution. From the plot also we can verify that the minimum energy required for formation of bound state among two electrons in a ladder like lattice is 2 , considering $t=1$.

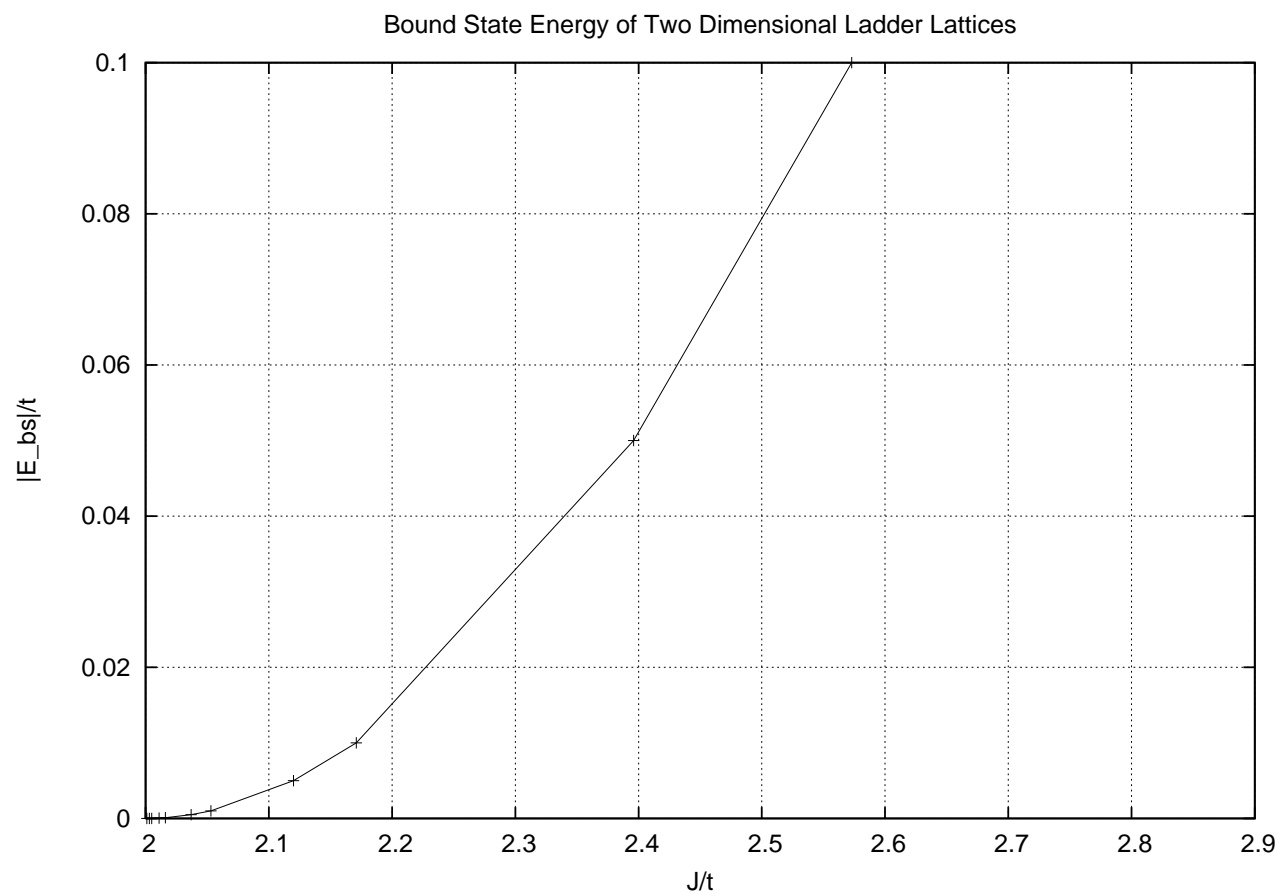


Fig 7

3.4 Three Dimensional Cubic Lattice:

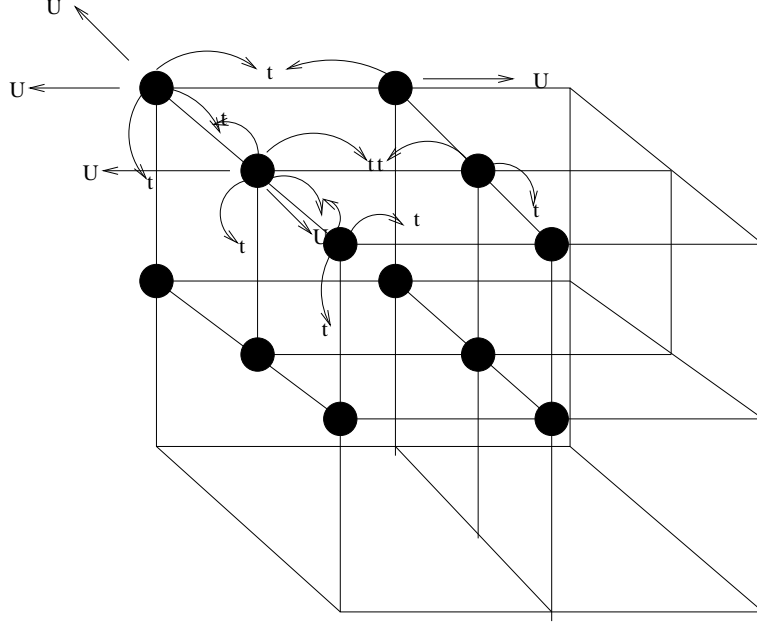


Fig 8

From eq.(9) considering that the lattice is isotropic ($Q=0$), we can write

$$\Phi_0(\mathbf{q}) = \frac{\frac{U}{N} \sum_k \Phi_0(\mathbf{k}) - \frac{1}{N} \sum_k J(\mathbf{q} - \mathbf{k}) \Phi_0(\mathbf{k})}{E - 2t(\mathbf{q})} \quad (41)$$

$$\Phi_0(\mathbf{q}) = \frac{\frac{U}{N} \sum_k \Phi_0(\mathbf{k}) - \frac{1}{N} \sum_k J(\mathbf{q} - \mathbf{k}) \Phi_0(\mathbf{k})}{E + 4t(\cos q_x + \cos q_y + \cos q_z)} \quad (42)$$

This equation can be written as follows:

$$C_0 = UC_0 I_0 - 2JC_x I_x - 2JC_y I_y - 2JC_z I_z \quad (43)$$

$$C_x = UC_0 I_x - 2JC_x I_{xx} - 2JC_y I_{xy} - 2JC_z I_{xz} \quad (44)$$

$$C_y = UC_0 I_y - 2JC_x I_{yx} - 2JC_y I_{yy} - 2JC_z I_{yz} \quad (45)$$

$$C_z = UC_0 I_z - 2JC_x I_{zx} - 2JC_y I_{zy} - 2JC_z I_{zz} \quad (46)$$

where

$$C_0 = \frac{1}{N} \sum_{\mathbf{q}} \Phi_0(\mathbf{q})$$

$$C_x = \frac{1}{N} \sum_k \cos k_x \Phi_0(\mathbf{k})$$

$$\begin{aligned}
C_y &= \frac{1}{N} \sum_k \cos k_y \Phi_0(\mathbf{k}) \\
C_z &= \frac{1}{N} \sum_k \cos k_z \Phi_0(\mathbf{k}) \\
I_0 &= \frac{1}{N} \sum_q \frac{1}{E + 4t(\cos q_x + \cos q_y + \cos q_z)} \\
I_x &= \frac{1}{N} \sum_q \frac{\cos q_x}{E + 4t(\cos q_x + \cos q_y + \cos q_z)} \\
I_{xx} &= \frac{1}{N} \sum_q \frac{\cos^2 q_x}{E + 4t(\cos q_x + \cos q_y + \cos q_z)} \\
I_y &= \frac{1}{N} \sum_q \frac{\cos q_y}{E + 4t(\cos q_x + \cos q_y + \cos q_z)} \\
I_{xy} &= \frac{1}{N} \sum_q \frac{\cos q_x \cos q_y}{E + 4t(\cos q_x + \cos q_y + \cos q_z)} \\
I_{yy} &= \frac{1}{N} \sum_q \frac{\cos^2 q_y}{E + 4t(\cos q_x + \cos q_y + \cos q_z)} \\
I_z &= \frac{1}{N} \sum_q \frac{\cos q_z}{E + 4t(\cos q_x + \cos q_y + \cos q_z)} \\
I_{zz} &= \frac{1}{N} \sum_q \frac{\cos^2 q_z}{E + 4t(\cos q_x + \cos q_y + \cos q_z)} \\
I_{zx} &= \frac{1}{N} \sum_q \frac{\cos q_z \cos q_x}{E + 4t(\cos q_x + \cos q_y + \cos q_z)} \\
I_{yz} &= \frac{1}{N} \sum_q \frac{\cos q_y \cos q_z}{E + 4t(\cos q_x + \cos q_y + \cos q_z)}
\end{aligned}$$

eq. (44), (45), (46), (47) can be written in a matrix form as follows:

$$\begin{pmatrix}
UI_0 - 1 & -2JI_x & -2JI_y & -2JI_z \\
UI_x & -2JI_{xx} - 1 & -2JI_{xy} & -2JI_{zx} \\
UI_y & -2JI_{xy} & -2JI_{yy} - 1 & -2JI_{yz} \\
UI_z & -2JI_{zx} & -2JI_{yz} & -2JI_{zz} - 1
\end{pmatrix}
\begin{pmatrix}
C_0 \\
C_x \\
C_y \\
C_z
\end{pmatrix} = 0 \quad (47)$$

J_c/t can be found out by vanishing of the determinant by choosing an energy E to be slightly between noninteracting 2 electron band.

$$\begin{vmatrix}
UI_0 - 1 & -2JI_x & -2JI_y & -2JI_z \\
UI_x & -2JI_{xx} - 1 & -2JI_{xy} & -2JI_{zx} \\
UI_y & -2JI_{xy} & -2JI_{yy} - 1 & -2JI_{yz} \\
UI_z & -2JI_{zx} & -2JI_{yz} & -2JI_{zz} - 1
\end{vmatrix} = 0$$

Since we are employing the constrain that there can not be any doubly occupied sites so considering $U \rightarrow \infty$, our vanishing determinant be as follows:

$$\begin{vmatrix} I_0 & -2JI_x & -2JI_y & -2JI_z \\ I_x & -2JI_{xx} - 1 & -2JI_{xy} & -2JI_{zx} \\ I_y & -2JI_{xy} & -2JI_{yy} - 1 & -2JI_{yz} \\ I_z & -2JI_{zx} & -2JI_{yz} & -2JI_{zz} - 1 \end{vmatrix} = 0 \quad (48)$$

Now because of lattice symmetry we can write

$$\begin{aligned} I_x &= I_y = I_z \\ I_{xx} &= I_{yy} = I_{zz} \\ I_{xy} &= I_{yz} = I_{zx} \end{aligned}$$

Also these lattice integrals can be written as:

$$I_x = \frac{1}{3} \left(\frac{1}{4t} - \frac{E}{4t} I_0 \right) \quad (49)$$

$$I_{xx} = -\frac{E}{4t} I_x - 2I_{xy} \quad (50)$$

So we need to find out I_0 and I_{xx} or I_{xy} .

Solution of Lattice Integrals

Previously mentioned lattice integrals are commonly known as lattice Green's function. The most general representation of lattice green's function is,[9]

$$\begin{aligned} G(s, l, m, n) &= \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{\cos lx \cos my \cos nz dx dy dz}{s - (\cos x + \cos y + \cos z)} \\ G(s) &= G(s, 0, 0, 0) = \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{dx dy dz}{s - (\cos x + \cos y + \cos z)} \end{aligned}$$

This integral defines a single valued analytic function $G(s)$ in the complex s -plane cut along the real axis from -3 to +3. in most physical applications one usually requires the limiting behavior of the Green function $G(s)$ as s approaches the real axis[10].

Another way we can write as[11]

$$\begin{aligned} \frac{1}{3} G(s) &= \frac{1}{3} \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{dx dy dz}{s - \frac{1}{3}(\cos x + \cos y + \cos z)} \\ G_1(s) &= \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{dx dy dz}{s - \frac{1}{3}(\cos x + \cos y + \cos z)} \end{aligned} \quad (51)$$

The series representation of the Green's function is[11]:

$$G_j(s) = \frac{1}{s} \sum_{n=0}^{\infty} \frac{p_n^{(j)}}{s^n} \quad (52)$$

where $j=1, 2, 3, 1 \leq |s| < \infty$ and

$$p_n^{(j)} = \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi [\lambda_j(\theta_1, \theta_2, \theta_3)]^n d\theta_1 d\theta_2 d\theta_3$$

Now for simple cubic lattice $\lambda_1(\theta_1, \theta_2, \theta_3) = \frac{1}{3}(\cos \theta_1 + \cos \theta_2 + \cos \theta_3)$ The recurrence relation for simple cubic lattice coefficient $p_{2n}^{(1)}$ is

$$36(n+1)^3 p_{2n+2}^{(1)} - 2(2n+1)(10n^2 + 10n + 3) p_{2n}^{(1)} + n(4n^2 - 1) p_{2n-2}^{(1)} = 0 \quad (53)$$

from eq. (52) and (53) $G_1(s)$ can be written as a solution of the linear third order differential equation

$$(s^2 - 1)(9s^2 - 1) \frac{d^3 G_1}{ds^3} + 6s(9s^2 - 5) \frac{d^2 G_1}{ds^2} + 3(21s^2 - 4) \frac{dG_1}{ds} + 9sG_1 = 0 \quad (54)$$

So $G_1(s)$ can be written as,

$$G_1(s) = \frac{1 - 9\xi^4}{s(1 - \xi)^3(1 + 3\xi)} \left[\frac{2}{\pi} \kappa(k_1) \right]^2 \quad (55)$$

where,

$$k_1 = \sqrt{\frac{16\xi^3}{(1 - \xi)^3(1 + 3\xi)}}$$

$$\xi = \xi(s) = \left(1 + \sqrt{1 - \frac{1}{s^2}} \right)^{-1/2} \left(1 - \sqrt{1 - \frac{1}{9s^2}} \right)^{1/2}$$

and $\kappa(k_1)$ is the complete elliptic integral of the first kind.

Also

$$G_1(1) = 3(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6}) \left[\frac{2}{\pi} \kappa((2 - \sqrt{3})(\sqrt{3} - \sqrt{2})) \right]^2 \quad (56)$$

So from this knowledge with proper adjustment of coefficients we can write:

$$I_0 = \frac{1}{12t} G_1(s) \quad (57)$$

Here we like to mention that elliptic integrals diverges for modulus of 1, the physical significance of the divergence in our work is the electrons are on the energy band therefore in our earlier analysis we had taken care of that divergence keeping our calculation just below the band, but here when we substitute our parameters as electrons are on the energy band we found the modulus is not 1 therefore there is no any sharp divergence of elliptic integral rather there is a local maxima, and we are returning with a numerical value of the integral on the band. Its a striking feature of the elliptic integral for simple cubic lattice. So from this knowledge we can evaluate I_0 . But one of the integral among I_{xx} or I_{xy} are still to be evaluated. To evaluate our integrals we had taken help from the recurrence relation of the Green function. With the knowledge of the recurrence relation for fcc lattice[12] and triangular lattice[13], we have constructed

the recurrence relation for simple cubic lattice. For nearest neighbour (6 nn for S.C) interaction only the recurrence is as follows:

$$G(l+1, m, n) + G(l-1, m, n) + G(l, m+1, n) + G(l, m-1, n) + G(l, m, n+1) + G(l, m, n-1) \\ = 2\delta_{l0}\delta_{m0}\delta_{n0} - 2sG(l, m, n) \quad (58)$$

where,

$$G(l+1, m, n) = \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{\cos(l+1)x \cos my \cos nz}{s + (\cos x + \cos y + \cos z)} dx dy dz$$

and so on, Let $l=1, m=0, n=0$ then

$$G(2, 0, 0) + G(0, 0, 0) + G(1, 1, 0) + G(1, -1, 0) + G(1, 0, 1) + G(1, 0, -1) = -2sG(1, 0, 0)$$

Due to the symetric structure of the lattice $G(1, 1, 0) = G(1, -1, 0) = G(1, 0, 1) = G(1, 0, -1)$ Hence, $G(2, 0, 0) + G(0, 0, 0) + 4G(1, 1, 0) + 2sG(1, 0, 0) = 0$

Adjusting the coefficients for our calculation,

$$I_{xx} = -\frac{E}{4t}I_x - 2I_{xy} \quad (59)$$

where, $I_{xx} = \frac{1}{8t}(G(2, 0, 0) + G(0, 0, 0))$, $I_0 = \frac{1}{4t}G(0, 0, 0)$, $I_x = \frac{1}{4t}G(1, 0, 0)$ Solving eq. (50) and (59) I_{xy} is determined.

$$I_{xy} = -\frac{E}{8t}I_x - \frac{1}{2}I_0 \quad (60)$$

Let us now summaries the lattice integral values:

$$I_0 = \frac{1}{12t}G_1(s), s = \frac{E}{4t} \\ I_x = \frac{1}{3}\left(\frac{1}{4t} - \frac{E}{4t}I_0\right) \\ I_{xy} = -\frac{E}{8t}I_x - \frac{1}{2}I_0 \\ I_{xx} = -\frac{E}{4t}I_x - 2I_{xy} \quad (61)$$

Substituting eq. (60) in eq. (48) and solving for J, the values are obtained as **2, 2, 7.88**.

4 RESULTS AND DISCUSSION:

In our entire work we were involved in finding out the critical values of J (J_c) for which bounstate formation of two electron system is possible, and our results obtained are as follows:

Lattice Type	J_c Values
One Dimensional Chains	2t
Two Dimensional Square Lattice	2t, 7.32t
Two Leg Ladder	2t
Three Dimensional Cubic Lattice	2t, 2t, 7.88t

Also we have plotted J_c/t Vs. $|E_{bs}|/t$ for one dimensional chain, two dimensional square lattice and two leg ladder.

For one dimensional chain like system has been already solved for $J=2t$ [14, 15].

For square lattice the critical value of $J=2t$ can seen in papers of Lin [1, 2]. In our work we are proposing that for two leg ladder lattice the critical value of J is $2t$, and it is quite desirable because two leg ladder is a simplified form of n leg ladder system which is nothing but a 2 dimensional system.

We are also proposing for the first time that for three dimensional lattice the critical value of J is 4.

Let us now try to understand the significance of the multiple value of two dimensional and three dimensional lattice for the basis of group theory.

Square Lattice

We know that the symmetries of a square lattice is represented by C_{4V} group. The character table for C_{4V} group is as follows:

Characters	E	C_4	C_4^2	C_4^3	m_x	m_y	σ_u	σ_v
$\chi^{(1)}$	1	1	1	1	1	1	1	1
$\chi^{(2)}$	1	-1	1	-1	-1	-1	1	1
$\chi^{(3)}$	1	-1	1	-1	1	1	-1	-1
$\chi^{(4)}$	1	1	1	1	-1	-1	-1	-1
$\chi^{(5)}$	2	0	-2	0	0	0	0	0

From the character table we can find out the irreducible representation of the group and the corresponding basis functions[16].

Irreducible Representation	Basis Functions
$\Gamma^{(1)}$	1
$\Gamma^{(2)}$	xy
$\Gamma^{(3)}$	$x^2 - y^2$
$\Gamma^{(4)}$	$xy(x^2 - y^2)$
$\Gamma^{(5)}$	(x, y)

The possible pairing symmetries correspond to these irreducible representation and to the basis functions. In case of square crystals the singlet orders are called s , $d_{x^2-y^2}$, d_{xy} and g . The corresponding basis functions are 1, $x^2 - y^2$, xy , $xy(x^2 - y^2)$. It is reasonable to classify order parameters as "s-wave like" and "d-wave-like". So in our analysis $J=2t$ corresponds to s-wave and $J=7.32t$ corresponds to d-wave[7].

Simple Cubic Lattice

It is known that the simple cubic lattice corresponds to O_h group. The character table for O_h group is as follows[17]:

Characters	E	$8C_3$	$6C_2$	$6C_4$	$3C_2(=C_4^2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	-1	-1	1	1	-1	1	1	-1
E_g	2	-1	0	0	2	2	0	-1	2	0
T_{1g}	3	0	-1	1	-1	3	1	0	-1	-1
T_{2g}	3	0	1	-1	-1	3	-1	0	-1	1
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	-1	-1	1	-1	1	-1	-1	1
E_u	2	-1	0	0	2	-2	0	1	-2	0
T_{1u}	3	0	-1	1	-1	-3	-1	0	1	1
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1

So the irreducible representation and basis functions for singlet pairing are[7]

Irreducible Representation	Basis Functions
$\Gamma_1(A_{1g})$	1
$\Gamma_2(A_{2g})$	$(k_x^2 - k_y^2)(k_y^2 - k_z^2)(k_z^2 - k_x^2)$
$\Gamma_3(E_g)$	$2k_z^n - k_x^n - k_y^n, k_x^n - k_y^n$ $n = 2; 4$
$\Gamma_4(T_{1g})$	$k_x k_y (k_x^n - k_y^n), k_y k_z (k_y^n - k_z^n), k_z k_x (k_z^n - k_x^n)$ $n = 2; 4; 6$
$\Gamma_5(T_{2g})$	$k_x k_y k_z^n, k_y k_z k_x^n, k_z k_x k_y^n$ $n = 0; 2; 4$

So in a cubic lattice, $\Gamma_1(A_{1g})$ represents s-wave pairing, $\Gamma_3(E_g)$ (for n=2) and $\Gamma_5(T_{2g})$ (for n=0) represents d-wave pairing[7]. Also $\Gamma_3(E_g)$ is doubly degenerate. So from the evaluated value of J, we can conclude that J=2t value corresponds to $\Gamma_3(E_g)$ representation and J=7.88t corresponds to $\Gamma_1(A_{2g})$ representation.

5 CONCLUSION AND FUTURE PROSPECTS:

The analytical result of J for simple cubic lattice is a new result. The result can be cross examined by bilayer consideration of the three dimensional cubic lattice. The bilayer consideration is analogous with the two leg ladder consideration. Physically it can be visualised that, n number of layers together is forming a three dimensional structure provided the separation between the layers is sufficiently small. So starting the calculation for bilayer one can extend the calculation to n number of layer which can give the similar result as of the three dimension. A natural extrapolation can be investigating superconductivity in these lattices and studying the phase diagram.

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